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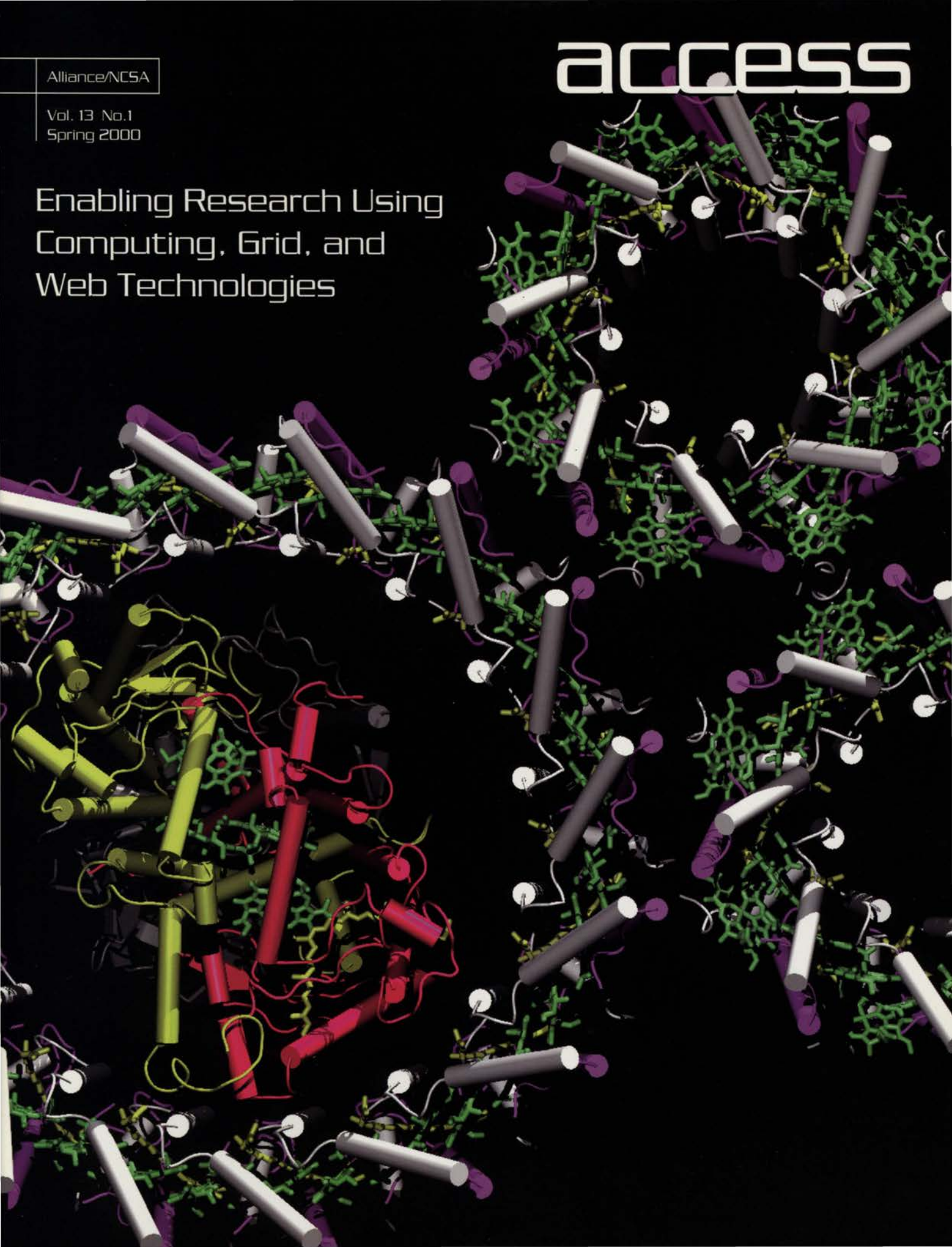
Enabling Research Using Computing, Grid, and Web Technologies



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Who we are

The National Computational Science Alliance (Alliance) is a partnership among more than 50 academic, government, and industrial organizations from across the United States to prototype an advanced computational infrastructure for the 21st century. This model infrastructure, called the Grid, will link together advanced supercomputers, visualization environments, and mass storage devices into a powerful, flexible problem-solving environment. This computing environment will be accessed via high-speed networks from anywhere in the country — eventually, the world.

The Alliance is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign with major support from the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

Cover
Top view of a bacterial photosynthetic unit. Outer rings of pigment molecules absorb light energy, which is then funneled to more central rings. Eventually the energy arrives at the reaction center—located inside the central rings—where a series of reactions drives metabolism. This visualization was created by the Theoretical Biophysics Group (TBG) at the University of Illinois at Urbana-Champaign. TBG is one of the Alliance's largest users of computational resources.

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access

Seeing the light

by Daniel Pendick

In the late 1980s, while still at the Technical University of Munich in Germany, Klaus Schulten found himself strapped for time on the handful of Cray supercomputers then available. To complete a particularly challenging computation—one simulating the structure and dynamics of cell membranes—Schulten thought he could speed things up by running the experiment on a parallel computer, which would divide the problem into separate tasks and solve them simultaneously.

Since no such machines were available to him, Schulten and his students built their own with 30 off-the-shelf processors. Schulten and his team have always done what it takes to harness leading-edge computer technology, even when they have had to roll up their sleeves and build the resources themselves.

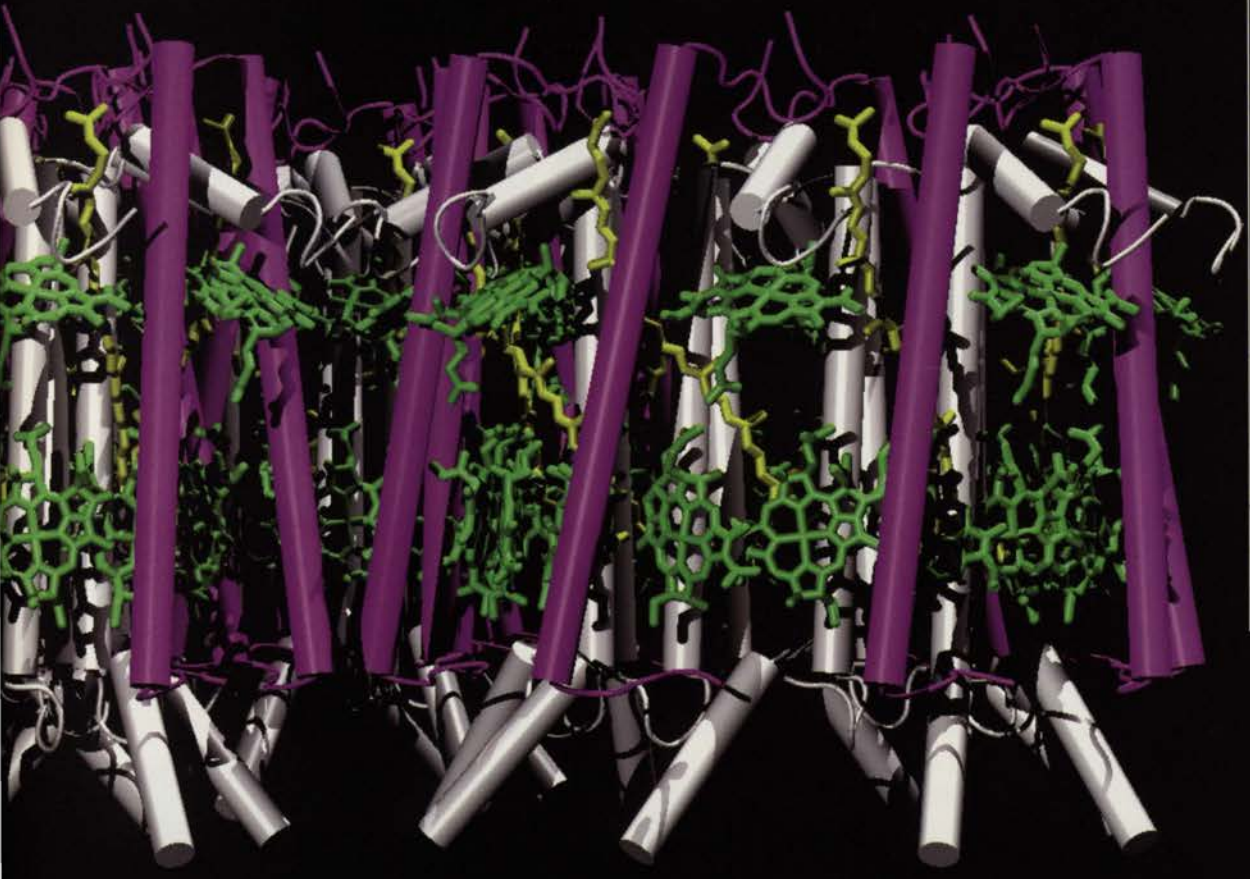
Now a professor of physics at the University of Illinois at Urbana-Champaign and a faculty member at the Beckman Institute, Schulten continues to study a variety of cellular activities—from how muscle proteins hold together to how single-celled organisms convert light to energy. Alliance supercomputers help him perform this research, but his drive for further innovation continues to shine through.

"I want to understand complete cellular machines, going from the atomic and molecular level all the way to large complexes involving hundreds of thousands to a million atoms," Schulten says. "That's what drives me to embrace the best computational resources."

One-stop computational science

While studying abroad at Harvard University in the late 1960s, Schulten discovered a new class of electron states that play an important role in photobiology. Since then he has continued to study the behavior of electrons in chromophores—complexes of molecules that enable plants, animals, and bacteria to interact with light. As he began to apply this theoretical understanding of atomic behavior in molecules to computer simulations, he captured the attention of the University of Illinois, which offered him a position in the physics department. In 1988 he arrived with 10 of his students in tow.

Klaus Schulten has always studied cellular activities of one kind or another. And he has always turned to the latest computer technology to further his research.



Side view of a bacterial photosynthetic unit. Outer rings of pigment molecules absorb light energy, which is then funneled to more central rings. Eventually the energy arrives at the reaction center—located inside the central rings—where a series of reactions drives metabolism. The L, M, and H subunits of the reaction center are shown in yellow, red, and gray, respectively. The beta-apoproteins are shown in magenta. The bacteriochlorophylls are shown in green, and the carotenoids are in yellow. This visualization was created with the Theoretical Biophysics Group's Visual Molecular Dynamics software package.

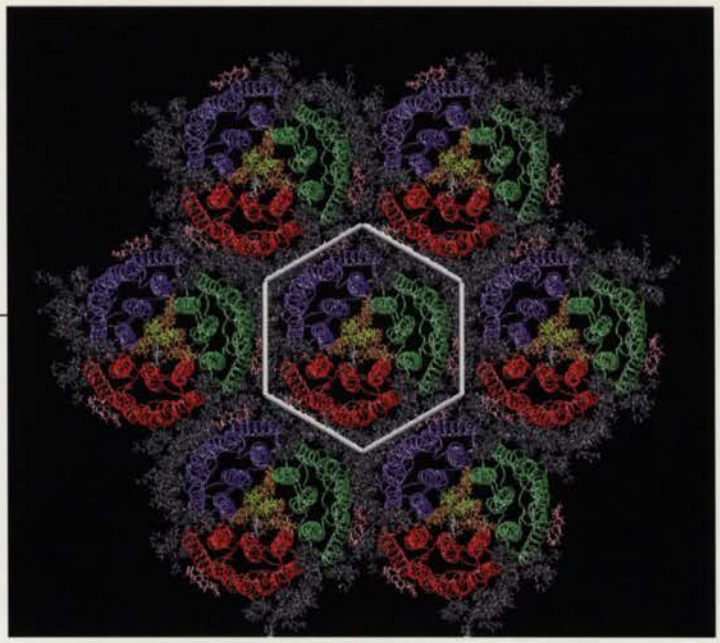
Schulten found a situation very different from what he was accustomed to in Germany. In Europe, he says, scientists could conduct their research at a handful of facilities with Cray supercomputers but received little support beyond that. NCSA, one of the first U.S. facilities to make supercomputers available to academic researchers, not only provided the computational horsepower to do large calculations but also offered high-performance workstations, programming staff, visualization programs, and other resources.

"You had not just a computer there, but a numerical and graphics laboratory. Not just material infrastructure but also intellectual infrastructure," Schulten explains. "I decided it was the place I needed to be."

At NCSA Schulten and his students increased the number of processors in their homemade parallel machine to 60. Their system was based on modular chips called transputers. Graduate students designed and constructed integrated circuit boards with six transputers and closely packed electronic memory chips. Schulten used the construction of the boards as an entry exam to his research team.

"Once the students finished their board they had to sign it, so I would know what boards came from which student," Schulten says. How well the boards worked "was the closest reflection I found of the student's later performance."

Schulten was using the transputers to characterize the structure of cell membranes. In contrast to a crystalline material such as ice or metal, membranes are a somewhat disordered amalgam of water and rod-shaped lipid molecules. Schulten's massive simulation essentially attempted to measure this disorder—calculating, for instance, how water molecules were distributed—with a degree of accuracy that matched experimental observations. The three-year simulation, published in 1993, involved about 30,000 atoms and, Schulten notes, was one of the first really large-scale simulations of a biological material.



Molecular model of a bacteria's "purple membrane." This image shows a trimer of bacteriorhodopsin proteins (center, surrounded by the white lines) and crystalline copies of the central trimer.

In 1989 Schulten founded the Theoretical Biophysics Group (TBG) at the University of Illinois at Urbana-Champaign (UIUC) so that computer scientists and basic researchers could work together in an equal partnership.

Such interaction is not necessarily the norm, says Laxmikant Kale, one of the two computer scientists from the University of Illinois on the TBG faculty. More typically, computer scientists may solve biological problems just to demonstrate the power of their computing methods, or a biology research group may hire a computer scientist just to take care of the computing chores. At TBG biology and computing are given equal roles in order to carry out large-scale research projects and develop software.

Today TBG consists of 40 faculty, students, postdocs, and staff members. Its external funding amounts to about $2 million per year. To meet their day-to-day needs, the group operates a network of workstations that functions as a high-performance parallel computer.

Though Schulten leads the group, his three faculty collaborators supervise TBG's many projects. Kale brings expertise in parallel computing and Web-based communication. Robert Skeel, the other UIUC computer scientist, specializes in algorithms. Todd Martinez, a UIUC professor of chemistry, is an expert on electronic structure and quantum dynamics.

New architectures

In the early 1990s, NCSA installed more powerful parallel hardware—Connection Machines from Thinking Machines Corp. Schulten was one of the pioneers on these machines and quickly became one of the heaviest users of the CM-2 system and its CM-5 successor.

"[Schulten's research team is] a good example of the sorts of people who jumped on new architectures and put the work into being able to utilize them," says Rick Kufrin, a senior research programmer at NCSA who worked with Schulten's group on both Connection Machines.

Colleagues credit Schulten's group with giving back to the research community the technology they have developed in pursuit of their basic research goals. For example, Schulten's group worked with NCSA programmers to develop a way to couple the Connection Machines—then the pinnacle of NCSA's computing resources—to SGI workstations. This connection allowed researchers to observe a simulation as it changed over time.

Their work evolved into a program called Visual Molecular Dynamics (VMD), which enabled researchers to visualize large and complex biomolecular structures. VMD later became part of MDScope, a fully integrated program for computational molecular dynamics released by Schulten's group in 1995. A version of VMD for Windows was released in January 2000.

The latest example of "shareware" from TBG is the Biological Collaborative Research Environment (BioCoRE). Schulten and his group are building this Internet-based system for collaborative research in molecular dynamics. BioCoRE will allow researchers and computer scientists to work together much as members of Schulten's local group do: sharing databases and code, viewing and analyzing simulation data, and archiving data and programs in a common site.

Kale says he hopes to make it possible to collaborate over the Internet, replacing conventional activities done on the telephone or in conference rooms. "What it really does is compete with the airline industry by making it unnecessary for researchers to fly to work together," Schulten notes.

The Theoretical Biophysics Group in the fall of 1999. Front row: Marilyn Lynch, Rosemary Braun, Margit Moellhoff, Jo Miller, and Gila Budescu. Second row: Gengbin Zheng, Klaus Schulten, Ana Damjanovic, Jim Phillips, Dorina Kosztin, David Hardy, Felix Autenrieth, Jerome Baudry, Thorsten Ritz, Barry Israelewitz, Angela Polino, and Ioan Kosztin. Back row: Robert Brunner, Robert Skeel, Charles Brown, John Stone, Justin Gullingsrud, Melih Sener, Sameer Kumar, Kirby Vandivort, and Hui Wang.

Bacteria harvest light, people harvest technology

With the availability of newer high-performance computers such as NCSA's SGI Origin2000, Schulten has continued the research on photobiology he began three decades ago at Harvard. His most recent work focuses on light-harvesting purple bacteria.

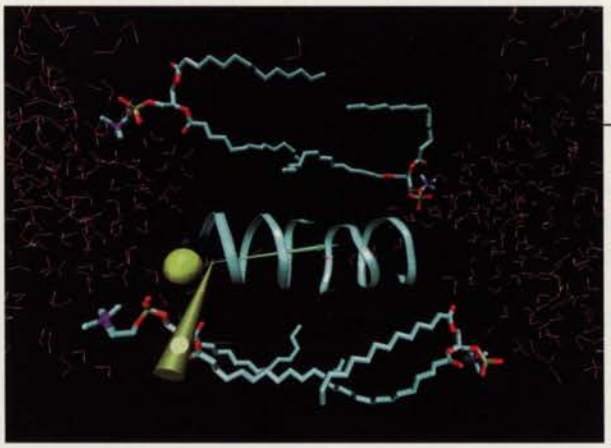
These single-celled organisms use their chromophores—blue and green pigments—to absorb photons and ultimately drive their metabolism. In the bacteria's cellular membrane, rings of pigment molecules serve as "light-harvesting antennae," Schulten explains. The light energy absorbed in the outer rings is funneled to more centrally located rings and eventually to a protein complex called the reaction center, which sets off a chain of reactions that drive the bacteria's metabolism.

The molecular machinery simulated by Schulten and his colleagues is the ultimate energy source for photosynthetic life. Being able to simulate the quantum electron states at the heart of photosynthesis not only confirms experimental data on the structure and function of these molecular machines but also deepens our understanding of the most fundamental biological system and explains how sunlight sustains life on Earth.

Along with all his contributions to photobiology, Schulten's colleagues also emphasize the "technological vision" that has enabled him to advance both computational science and his basic research goals. This vision has helped him attract talented students and collaborators.

"Working with Klaus's group has been one of the most rewarding collaborations I've had," Kufrin says. "They're pushing the edge, but there's also a kind of neat excitement when you work with them. I think that excitement comes from Klaus."

Schulten, however, insists that it's really the crew that gets the boat to its destination—an attitude that shows in the way TBG works and in Schulten's efforts on the BioCoRE collaboratory. "It all works," he says, "only because I am very fortunate to have a good team."



A potassium ion being pulled through an ion channel using a haptic force-feedback controller. The haptic device allows the researcher to feel the tug and repulsion of molecules during a simulation.

Hands-on molecular dynamics

One day John Stone, a research programmer in the Theoretical Biophysics Group (TBG), went shopping for joysticks. He wasn't trying to help graduate students make it through the night with a little help from Nintendo; Stone needed a joystick to grab onto virtual molecules and see how much of a fight they put up when dragged through simulated cell membranes.

Welcome to Interactive Molecular Dynamics (IMD), TBG's latest modeling software that combines visualization and simulation in real time. IMD adds a key new tool to molecular modeling that lets researchers manipulate and receive feedback from computer models using a force feedback joystick known as a haptic device.

Achieving the speed necessary for IMD projects requires massively parallel computing resources and a highly efficient and scalable simulation program. During a recent capability computing run on a 256-processor configuration of NCSA's SGI Origin2000 supercomputer, TBG used their widely distributed NAMD2 software to complete the first proof-of-concept IMD projects and feel the tug and pull of simulated molecules. Once IMD moves beyond the test phase, it will allow researchers to manipulate biomolecular systems of up to 10,000 atoms while investigating computer simulations of drugs docking to receptor targets, for example, or of ions permeating through membrane channels.

TBG also used its month of Origin2000 time to complete a series of more traditional batch mode steered molecular dynamics simulations. In a batch mode steered molecular dynamics simulation, the forces that researchers want to use to manipulate a biomolecular system need to be completely defined in the code before a run. Feedback through a haptic device is not possible.

One project explored atomic force microscopy experiments that stretched the protein titin-a key component of muscle tissue-to investigate the elasticity of muscle and its failure in heart disease.

Another simulation focused on ion channels in membranes. Ion channels permit specific charged molecules, or ions, to enter a cell. By studying how different ions move through the channels of a simulated cell, TBG researchers hope to better understand how nerve cells fire.

According to Schulten, IMD is about using and developing the investigator's intuition in manipulating biomolecular machines. Haptic devices make the process a lot more like tinkering to repair a jammed clock mechanism.

"With IMD you can probe, you can see where it's easy to pull, where it's hard to pull, and in this way you slowly develop your intuition about the process," Schulten explains. "There's lots of wisdom to be gained from feeling and controlling the tiny movements of cellular machines."

The Theoretical Biophysics Group receives funding from the National Institutes of Health, the National Science Foundation, the Roy J. Carver Charitable Trust, and the University of Illinois.

http://access.ncsa.uiuc.edu/CoverStories/MolPhotodynamics

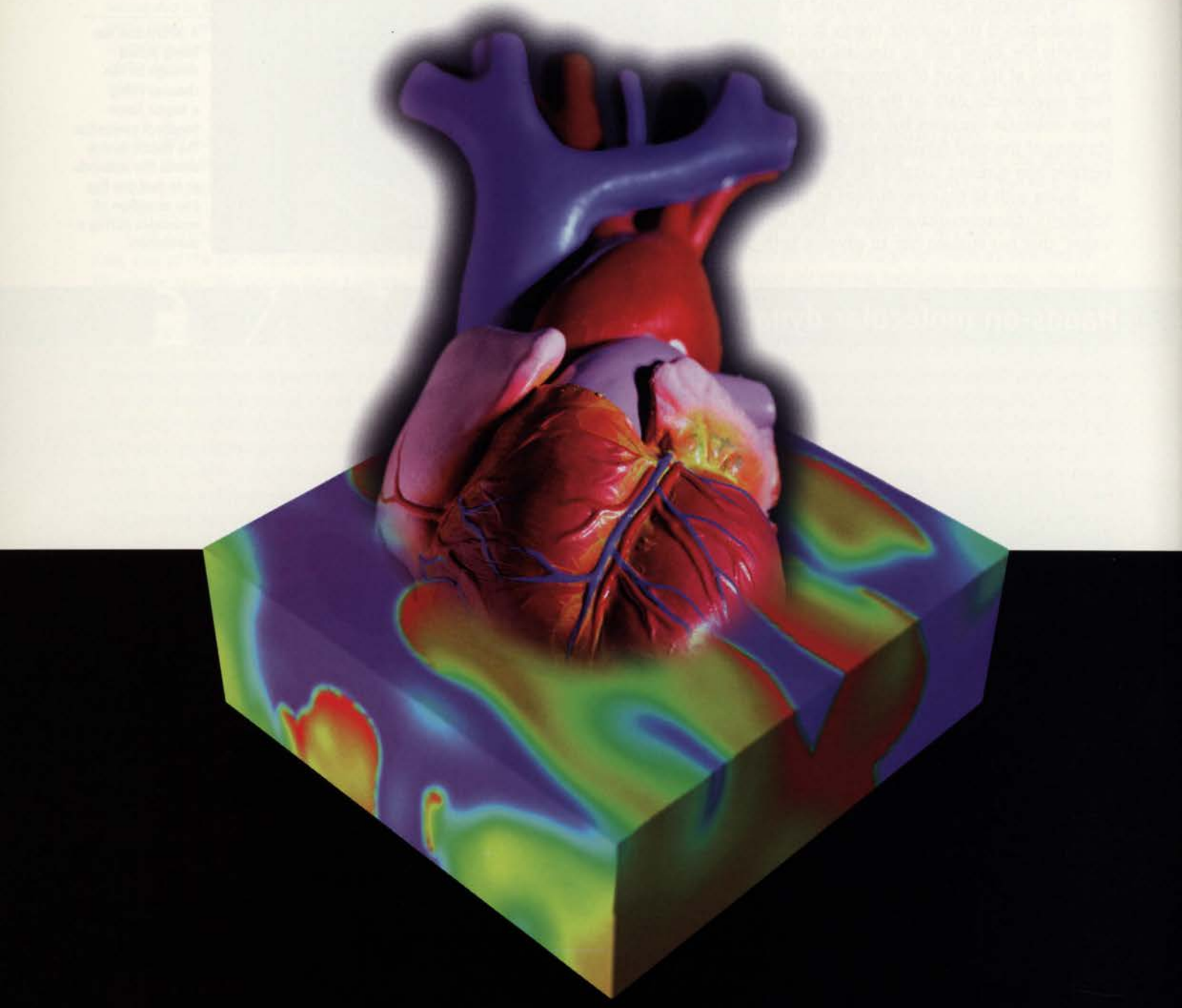
For more information about this research project, see the following URLs:

http://www.ks.uiuc.edu/
http://www.ks.uiuc.edu/Research/mdscope/
http://www.ks.uiuc.edu/Research/psu/psu.html
http://www.ks.uiuc.edu/Research/vmd/
http://www.ks.uiuc.edu/Research/collaboratory/
http://www.ks.uiuc.edu/Overview/gallery/structure.shtml
http://www.ks.uiuc.edu:554/ramgen/sureLH2.rm

Chaos and the fibrillating heart

Today's heart simulations may someday make traumatic jolts from heart defibrillators a thing of the past.

by Patricia Craig



The sound of a beating heart—the familiar lub-dub that accompanies our daily rhythms—can suddenly, with no warning, go wrong. The heart's electrical signals go haywire, the pumping cycle is disrupted, and the heart quivers, or fibrillates, uncontrollably. Unless corrected, death results in a matter of minutes.

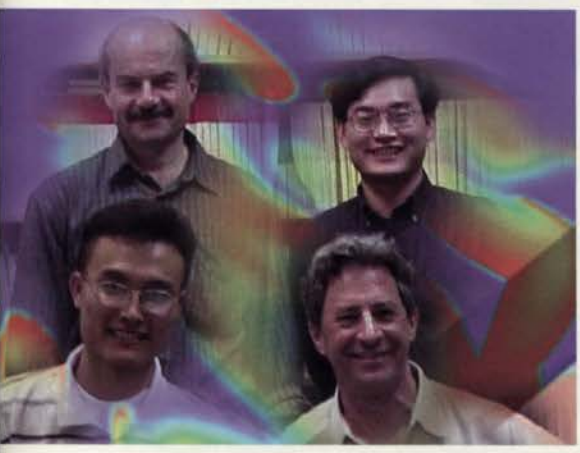
The leading cause of sudden cardiac death in the United States, ventricular fibrillation kills 350,000 people every year. Occurring most often in older patients with damaged heart tissue, it can also strike healthy young adults with no history of heart disease. The only known antidote is a powerful, potentially damaging jolt from a defibrillator, the ever-present electrical paddles that accompany the call to "Clear!" on emergency medical television shows.

Defibrillators are found not only in hospitals but also in airplanes, airports, and, increasingly, implanted in patients' chests. While advocates would place a set of paddles in every home, some scientists believe that defibrillators are not the final answer.

"A defibrillator is what you use when you are clueless," says cardiac physiologist Alan Garfinkel.

Garfinkel, a professor in the departments of medicine and physiological science at the University of California at Los Angeles, is anything but clueless. His research group's models of fibrillation in simulated heart tissue give him the opportunity to explore the malady and its causes. Created using Alliance supercomputers at the Maui High Performance Computing Center, the models also offer hope for new and better treatment.

"Alan's elegant work offers the possibility of designing interventions to prevent fibrillation from occurring at all," says Kenneth Stein, a professor of cardiology at Cornell University Medical College.



Clockwise from bottom right: Alan Garfinkel, Zhilin Qu, James Weiss, and Jong Kil, University of California at Los Angeles

Spiral waves

Electrical signals propagate through normal heart tissue in successive waves of electrical activity, like a wildfire propagating through a forest. A group of what are known as pacemaker cells set off a small excitation that causes a contraction of the heart muscle that pumps blood. When the contraction passes, a period of relaxation is required to prepare for the next wave. This orderly rhythm happens hundreds of times each hour.

Fibrillation can result from a bump in the rhythm, an abnormality called an ectopic contraction (EC). An EC is a self-excited muscle cell that fires off an unbidden volley of excitation. While ECs can be provoked by drugs—especially cocaine—and occur most often in damaged tissue, Garfinkel says that the normal heart experiences at least one small EC every hour. If an EC happens to occur at the back of a normal receding wave, the current radiating from it runs into tissue that the normal wave has already passed. This tissue is in a recovery phase and is not ready to be excited again.

ECs are normally too small to do any damage, and the radiating current dissipates. Occasionally, however, they are large enough, or enough ECs happen in quick succession, to cause problems. The wave curls back on itself—repelled by the resting tissue—and assumes a spiral shape. This spiral wave can circle around itself again and again, like a cat chasing its tail. The result is a rapid heartbeat called ventricular tachycardia. The ordinary palpitations and rapid heartbeats we all experience occur in the upper chambers of the heart, the atria, and are not nearly as dangerous.

Ventricular tachycardia often decays into fibrillation as the spiral wave quickly becomes unstable and breaks up spontaneously into more spiral waves. Within seconds a massive number of waves is present. They reenter tissue they've already traversed, loop back on themselves, and cause irregular and disordered behavior—the hallmark of fibrillation.

Such turbulence is also the hallmark of chaos.

Two years ago, with Peng-Shen Chen and Hrayr Karagueuzian, both of Cedars Sinai Medical Center, and UCLA cardiologist James Weiss, Garfinkel found that the onset of fibrillation in a dog's cardiac tissue occurred not in a random fashion but according to the rules of chaos theory. Although the name suggests otherwise, chaotic systems follow distinct, albeit complex, patterns that can be described with nonlinear mathematics.

Chaos is everywhere—in a dripping faucet, the population dynamics of butterflies, the behavior of an airplane in flight. The chaos that Chen, Karagueuzian, and Garfinkel saw in the dog heart was the first transition to chaos ever described in a medical setting, and it was very welcome news. Because the onset of fibrillation follows rules, the simulation models Garfinkel and his colleagues were making had the potential of leading to predictive, and thus therapeutic, outcomes.

"Had it turned out not to be chaotic behavior," Garfinkel says, "we'd have had to basically close the book and say, 'We'll just have to build better defibrillators.'"

55 million variables

Garfinkel modeled his original simulations in two dimensions on the DEC Alpha workstations in his lab. As he pushed for greater realism, he had no choice but to turn to supercomputers, which can handle the computationally intensive algorithms required for the necessary simulations in three dimensions.

Scroll wave breakup in a block of cardiac tissue. Reentrant tachycardia can break up into the turbulent, chaotic state known as ventricular fibrillation, the principal cause of sudden cardiac death. This simulation, like the scroll wave shown above, was run in a 320 x 320 x 60 lattice with variables updated every .01ms in a 1000 ms run.

A simulated spiral wave (called a scroll wave when modeled in 3D) in a block of cardiac tissue. In normal heart muscle, a wave of excitation passes though the muscle, creating the wave of contraction that pumps the blood. In pathological conditions, this wave can turn upon itself to become an arrhythmia. Here, the wave has turned upon itself to become a reentrant tachycardia, itself a serious medical condition. This simulation was done in a 320 x 320 x 60 lattice of cardiac cell models. Each cardiac cell is modeled by a seven-variable ordinary differential equation with a timestep of .01 millisecond (ms). The variables are each updated every .01 ms during the course of a 1000 ms run.

The smallest reasonable amount of heart tissue that will support a spiral wave, he explains, measures 300 x 300 x 100 computational cells. Each of those cells must be described by at least six variables—ion levels and voltage, for example—making for about 55 million variables. Each variable is updated every one-hundredth of a millisecond, and each update is dependent on the previous outcome. In addition, a host of other feedback systems that the researchers adapted from traditional mathematical and electrophysiological equations are built into the algorithms.

To model a single wave—about one second's worth of simulated action—Garfinkel and his colleagues require 18 hours on a 44-processor IBM SP2 supercomputer cluster. The group uses SP2s both at the Maui High Performance Computing Center, an Alliance Partner for Advanced Computational Services, and at the San Diego Supercomputing Center, leading-edge site of the Alliance's sister program, the National Partnership for Advanced Computational Infrastructure.

At the outset the big question was how to prevent a spiral wave from breaking up and propagating. After changing key variables in some 20 simulations, Garfinkel and his team found that the value of only one variable was making a huge difference in spiral wave stability. This variable, the restitution property, reflects the amount of time a cell must rest before contracting again. If you stimulate a heart cell without having given it a chance to rest properly, Garfinkel explains, the sodium, potassium, and calcium ions that maintain the electric potentials can't flow fast enough to bring the cell back to equilibrium after the current has passed through.

By giving their computer models a drug that changes the timing of the ionic currents and allows the cells to recover faster, the researchers found that the spiral waves simply fizzled out.

Recipe for a drug

The therapeutic potential of this result is clear: Develop a drug that allows the cells to recover more quickly in the prefibrillation period so that tachycardia is prevented from decaying into full-blown fibrillation. The trauma of shocking a heart back into its normal rhythm using a defibrillator is avoided.

Most antiarrythmia drugs today work—if they work at all—by blocking ionic channels. A major problem, says Stein, is that these drugs aren't specific; they block the same channels in all other cells in the body at the same time. "It's like using a baseball bat as a flyswatter."

Garfinkel's hope is to develop a new class of drugs that works not by blocking ionic channels but by changing the time dynamics of current flow. His future plans include simulations of atrial fibrillation, a phenomenon that differs from ventricular fibrillation mostly in lethality. The atria contribute very little power to the ventricle's main function of pumping blood. When they are out of commission the heart still works at 80 percent efficiency. However, blood clots formed in pooled blood in the quivering chambers still represent a significant danger.

Scientists predict that both atrial and ventricular fibrillation will claim more victims as the population ages, and Garfinkel is convinced that atrial fibrillation will be "the disease of the double Os."

"The potential for Alan Garfinkel's work is huge," says Steven Evans, chief of the electrophysiology section at Beth Israel Medical Center in New York City. "Knowing the mechanisms behind fibrillation will not only provide better treatment, it will help us predict which patients are most at risk. It can potentially impact hundreds of thousands of lives."

This research is supported by the National Institutes of Health and the Western States Affiliate of the American Heart Association.

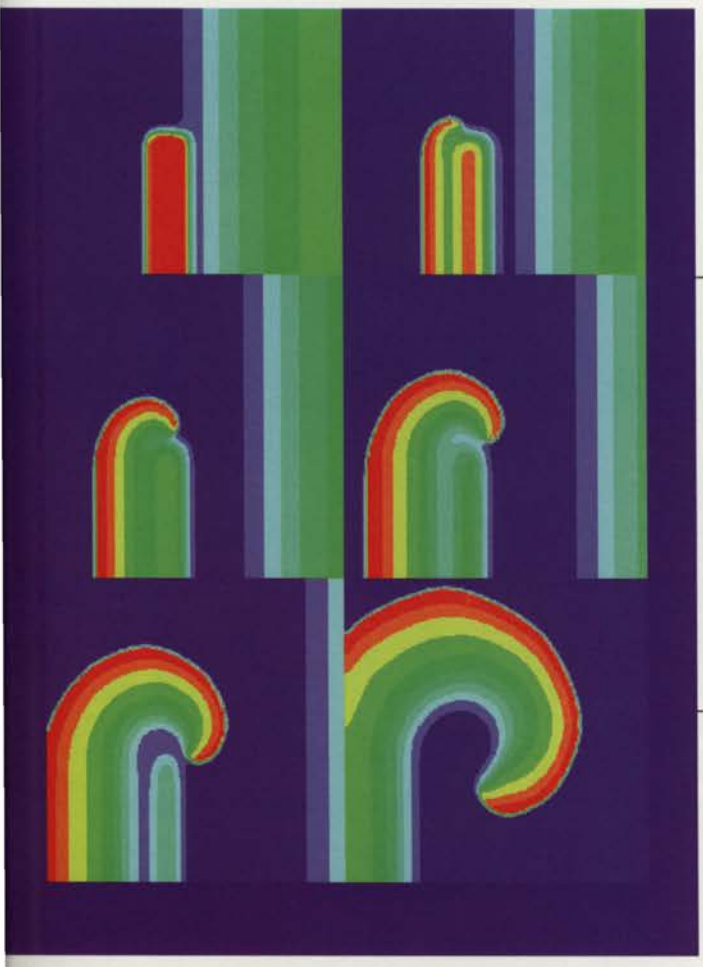
http://access.ncsa.uiuc.edu/CoverStories/HeartChaos/

For more information about this research project, see the following URLs:

http://www.mhpcc.edu
http://heartlab.mednet.ucla.edu/
http://www.BethIsraelny.org/

Team members

Alan Garfinkel
James Weiss
Zhilin Qu
Jong Kil



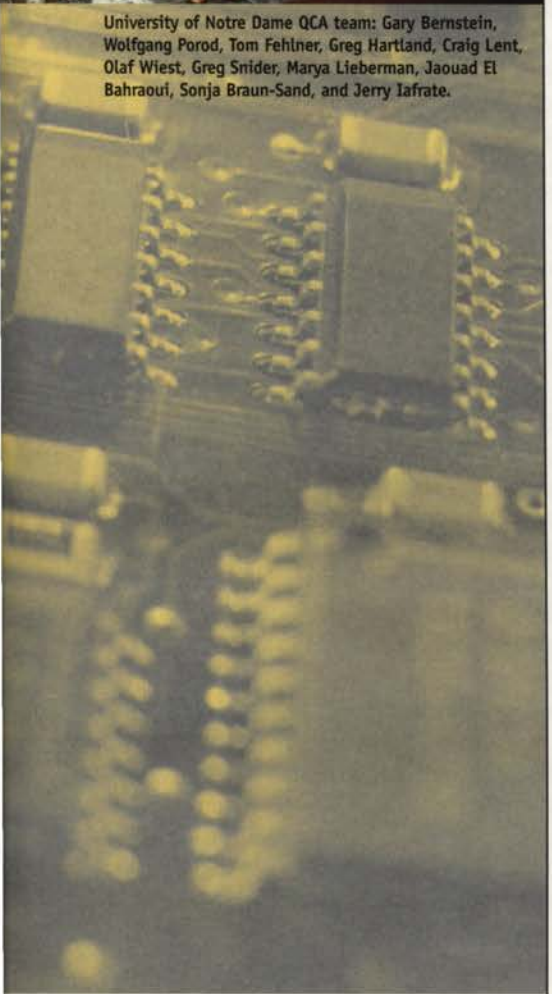
Formation of a spiral wave by an ectopic contraction. This earlier 2D model of cardiac tissue was constructed as a 300 x 300 lattice of cells, each cell modeled by a seven-variable, ordinary differential equation. It shows six successive snapshots of voltage distribution as a spectrum of color over the tissue. Blue (the resting state) has the lowest voltage and red has the highest. In the upper left panel, a wave of excitation has passed from left to right. Its highest values have already passed through the region so that only the greens and blues of partial recovery remain. The bright red bar is a new, second excitation that has risen ectopically in the partially recovered tail of the previous wave. The subsequent panels show its evolution. The wave has propagated slowly in the partially recovered region on the right and faster in the fully recovered region on the left, thus introducing curvature into the wavefront.

small talk

Quantum-dot Cellular Automata may someday replace transistors at the heart of microelectronics. Scientists at the University of Notre Dame are just beginning to develop these miniature marvels.

by J. William Bell

University of Notre Dame QCA team: Gary Bernstein, Wolfgang Porod, Tom Fehlner, Greg Hartland, Craig Lent, Olaf Wiest, Greg Snider, Marya Lieberman, Jaouad El Bahraoui, Sonja Braun-Sand, and Jerry Iafrate.



In 1971 Intel's top-of-the-line microprocessors had 2,300 transistors—just over 2,000 on/off switches that carried a computer's binary signal and made all of its computation possible. The microprocessors in today's desktop computers, while still not much bigger than a postage stamp, have more than seven million transistors. The early microprocessor performed about 60,000 calculations per second while today's performs hundreds of millions.

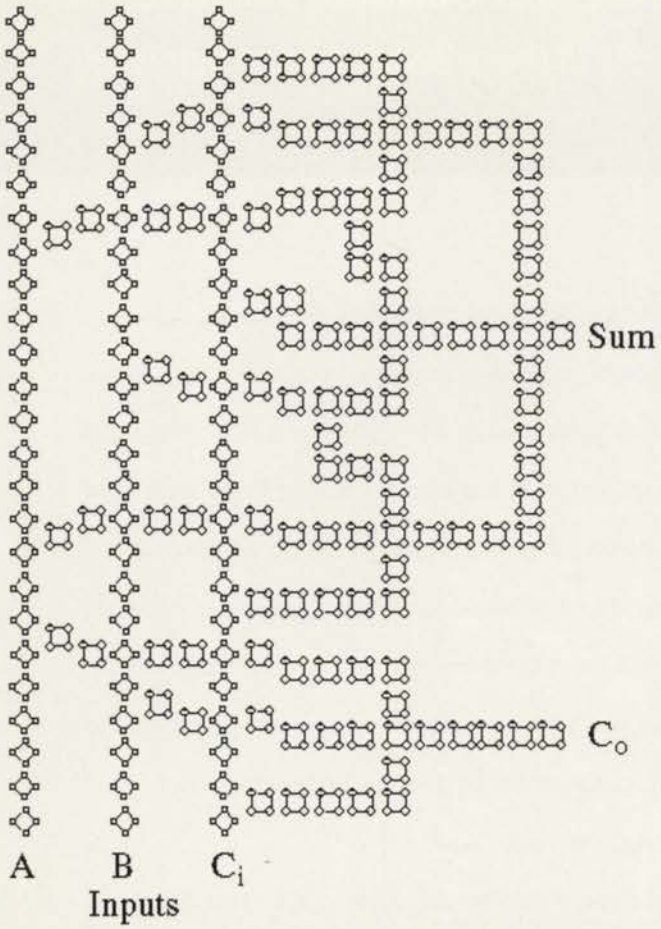
But the trend of the incredible shrinking transistor—and the ever more powerful computer that goes with it—can't continue forever. Many researchers are not confident that transistors can shrink much further at all, much less keep pace with the staggering historical pattern.

"The transistor and silicon roadmap does have an end," says Gerald Iafrate, director of the Center for Nano Science and Technology at the University of Notre Dame. "We're looking at devices that reach beyond the end of that growth."

Quantum-dot Cellular Automata, or QCA, is extending that reach.

QCA is a tiny technology with huge implications. Microprocessors the size of a grain of sand with the power of 100 desktop workstations and computer memory that is incredibly cheap but uses next to no power are just a couple of possible breakthroughs that people mention when they discuss the technology.

QCA theory is less than a decade old, and the first computers to use it are likely a couple of decades away. Nonetheless, an interdisciplinary team of Notre Dame scientists using NCSA's SGI Origin2000 supercomputer and funded by the Defense Advanced Research Projects Agency's Moletronics project is already putting results behind the small talk.



A set of QCA cells that adds a series of inputs designed by Craig Lent and P. Douglas Tougaw created with a set of QCA cells. The interactions between QCA cells arranged in a given pattern determine the set's logical function.

QCA Q-and-A

Where there were once transistors, QCA technology contains sets of identical square cells, each only one ten-millionth of an inch on a side. Each cell contains two extra electrical charges that can move about the cell. At each of the cell's corners is a "dot" where the charges can be located. The charges repulse one another through a force known as Coulomb interaction. This repulsion means that they get as far away from one another as they can, leaving only two possible sets of locations for them. The particles always inhabit one of the cell's two sets of opposite corners.

The fact that only two stable arrangements of the cell can exist allows information in a QCA device to be treated just as in a traditional electronic device. An individual cell acts as a switch, and the ones and zeros of binary code are represented in the switch's two positions. The position of the charges in one cell is influenced by the position of the charges in neighboring cells, again through Coulomb interaction. This influence causes the cells' states to change, and single bits of data are processed and passed down the line.

As with transistor-based systems, the pattern and arrangements of a set of cells determine the set's function, such as whether the cells add a series of inputs, invert a signal, or simply carry the signal like a wire carrying a current. Unlike a transistor however, all the components—the cells—are identical and differ only in how they are arranged with their neighbors.

Last year the Notre Dame research team announced that they had created a functioning logical switch in a QCA cell that used one pair of electrons as the charges. However, the switch required temperatures near absolute zero. Now the Notre Dame team is focusing on using single complex molecules as QCA cells. Different states of the electrons in the molecules would be used to encode information. This system will theoretically work at room temperature.

"The theory has been around for a while now, and the first successes have been made. But we've arrived at figuring out how to actually do all this, and that's how the chemists came into it," says Olaf Wiest, an assistant professor of chemistry at Notre Dame. Wiest, postdoctoral research associate Jaouad El Bahraoui, and graduate student Sonja Braun-Sand are using the Origin2000 to model molecules that could be used in molecular-scale QCA devices.

A molecule that's just right

The perfect molecule for QCA is a finicky character—a regular Goldilocks of nanoscience—and its vagaries must be perfectly understood before it can be used. If it says "too hot" when everyone expects it to say "too cold," the system doesn't work, resulting in a sensor that doesn't turn on or a computer that corrupts its own data.

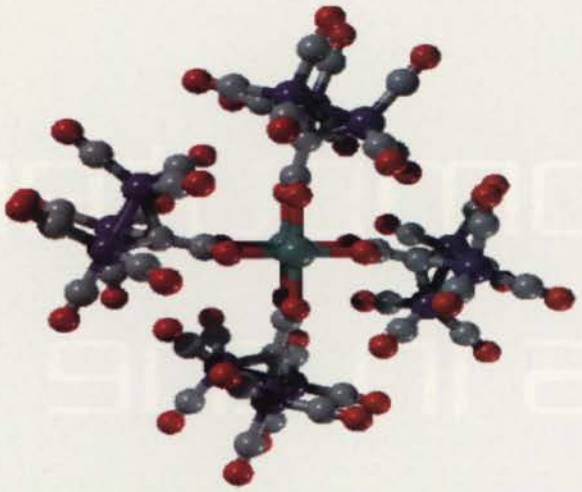
"We have to understand the differences between the two states that the individual QCA molecules have, how they change between those two states, and how individual cells influence one another," Wiest says.

In other words, they have to know when and why the charges are going to change and the switch is going to flip from a binary one to a binary zero. They also have to pick a molecule that will flip when they want it to, a molecule that will function within a very strict range of variables that includes temperature and energy levels.

"It has to be just right," Wiest says, "If the activation energy—the level at which Coulomb repulsion causes it to change states—is too high, it will never change and won't pass any information. If it is too low, it will simply flip randomly."

Wiest and El Bahraoui are using a 16-processor configuration of the Origin2000 to perform ab initio calculations on compounds containing transition metals, such as cobalt and ruthenium, that are likely candidates for use in molecular-scale QCA technology.

Ab initio methods use no approximations in modeling the molecule and provide a very accurate representation without any adjustable parameters. It is "the current state of the art in modern electronic structure theory," according to El Bahraoui. The results will, of course, allow researchers to make predictions



A large transition metal complex–$Mo_2[(CO)_9Co_3CCO_2]_4$–on which QCA technology may someday be based. Red represents oxygen, blue is colbalt, green is molybdenum, and gray is carbon.

about the nature of the molecules. The results will also help the researchers develop methods of simplifying and improving the calculations and allow researchers to begin modeling the behavior of systems of the adjacent cells that compose complete circuit devices.

The calculations—which are performed using Gaussian™, HONDO, and QCHEM software packages—are much larger than those traditionally calculated using ab initio methods. The calculations operate using over 1,500 basis functions, equations that represent the molecule in the calculation's algorithm.

"These calculations are very, very huge and can take anywhere from a day to several weeks to run for a single molecule," says El Bahraoui. "But a few years ago, they couldn't be done at all on transition metal compounds of this size."

Continual conversation

A standard computer chip that now holds seven million transitors may hold as many as one trillion QCA devices. Because QCA relies on Coulomb interaction rather than electrical current to pass a signal, QCA uses minimal power and produces minimal heat. QCA is also considered a brilliant match for image processing systems, where myriad calculations are required for each pixel. The list of potential applications goes on and on.

But the list of challenges is just about as lengthy. A new fabrication process will have to be developed for QCA devices. Once the molecules are designed and understood through computer simulations, they must be synthesized. And getting data in and out of a single molecule still requires big, expensive machinery that isn't usable in everyday applications.

Faculty at Notre Dame are addressing all of these problems. But in the meantime, they have to address one another, too.

"There's a continual conversation and translation between the fields," says Marya Lieberman, an assistant professor of chemistry at Notre Dame who is working on the QCA project.

That conversation is more than just small talk and as important as any other aspect of the research, according to Gerald Iafrate. "You can't stress integration enough," he says, "You've got to have a strategic target and make sure that everyone works toward it. You can't just work on your personal widget."

This research is supported by the Defense Advanced Research Projects Agency.

http://access.ncsa.uiuc.edu/CoverStories/MolElectronics/

For more information about this research project, see the following URLs:

http://www.nd.edu/~ndnano/
http://www.nd.edu/~qcahome/
http://www.darpa.mil/mto/

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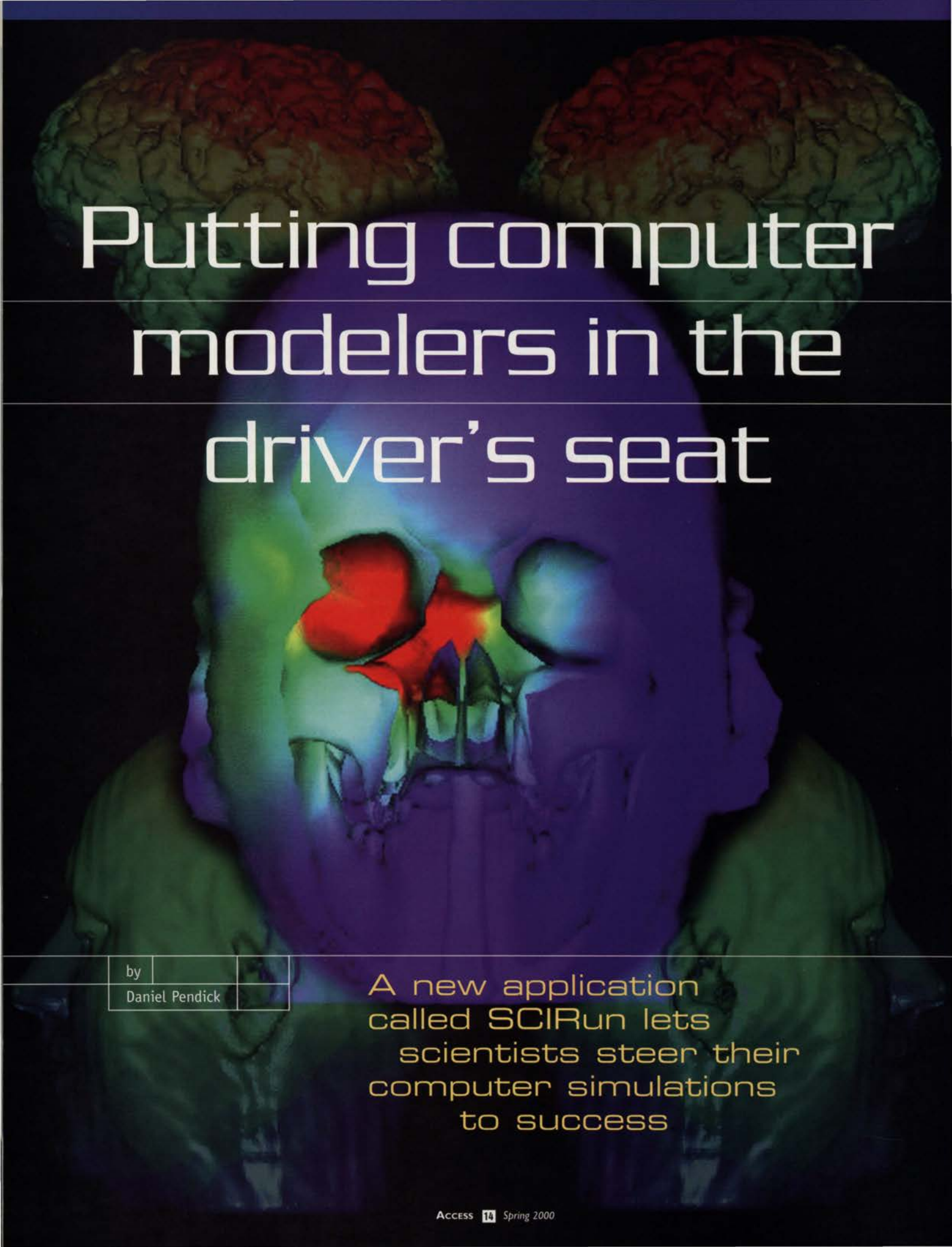


Putting computer modelers in the driver's seat

by
Daniel Pendick

A new application called SCIRun lets scientists steer their computer simulations to success

Though most scientists would prefer to pilot their computer simulations with the deftness of an Indy 500 driver, too often they end up feeling like crash test dummies: After much preparation, they rev up their simulations and then watch helplessly as those simulations hit unexpected obstacles and crash, sending the scientists back to the starting line.

Chris Johnson hopes to change all that. Johnson is the director of the University of Utah's Center for Scientific Computing and Imaging and a member of the Alliance Distributed Computing team. He and his colleagues have created a computational workbench that combines modeling, simulation, and data visualization into a single system. Dubbed SCIRun (pronounced ski run), it allows scientists to interact with computations while they are still en route. SCIRun helps provide a pothole-free path for scientists as they build models, run simulations, and visualize the results.

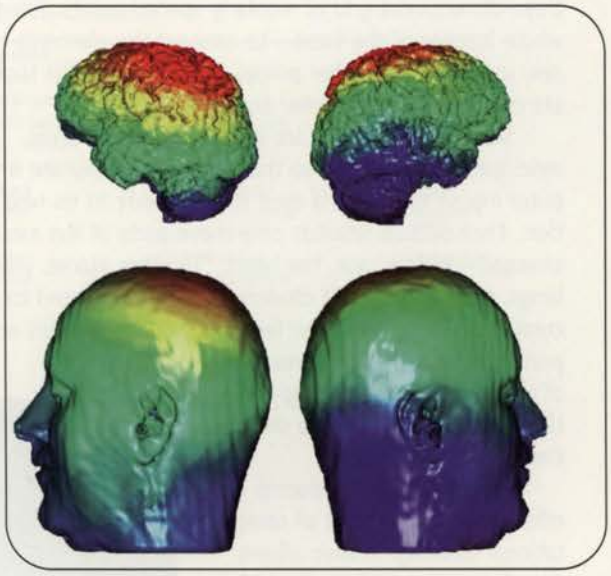
Chris Johnson, University of Utah

Three in one

In the mid-1980s Johnson developed a simulation of the bioelectric fields generated by a beating heart. He and his colleagues had to combine three tasks: building a computational model of the chest and heart, running a simulation of the heart's electrical activity, and then visualizing the data that the model produced.

"Traditionally each of these tasks required different computational tools that didn't talk to each other very well," Johnson explains. "We would spend all this time moving the data from the modeling tools to the simulation tools to the visualization tools, usually changing the data file format several times."

The solution, Johnson thought, was to create a single, integrated tool that would eliminate the mismatches and file management chores. Such a system would allow a user to monitor the simulation and intervene in midstream. This approach is now known as computational steering.



Visualization of electrical voltage on the surface of the brain and scalp. Red indicates positive voltage, blue indicates negative voltage, and green indicates voltages of approximately zero. Visualizations of the brain (top) were computed using high-resolution EEGs along with head and brain geometry information from MRIs. Such studies of brain electrophysiology may lead to a better understanding of brain abnormalities as well as such thought processes as language use and reasoning.

In the early 1990s Johnson kicked off the development of SCIRun. The project got a major jump start when graduate student Steven Parker joined the Utah lab. "I thought I would have a long succession of graduate students working on little pieces of the project," Johnson recalls. But Parker took the lead on the computational steering project and began to reengineer the heart and torso model into the program that evolved into SCIRun. Parker has since completed his PhD and remains at the Center for Scientific Computing as a staff scientist.

The heart of computational steering

First Parker built interactivity into the heart model. At the time, Johnson's lab was developing a version of the model needed by researchers from Siemens-Pacesetter, Inc., of Sylmar, CA, to develop an implantable defibrillator, a miniature version of the device used to shock a misfiring heart back into normal rhythm. An important aspect of the design was finding the right spot on the heart surface to place two electrodes that are the equivalent of the two paddles that deliver the shock in the larger version.

Parker found that changing the location of an electrode meant rewriting a file in the application to specify the electrode's new location. Then he had to rebuild the mesh—a three-dimensional grid of regularly spaced points filling the whole interior of the torso—to connect the electrode in its new location to all other points. Rewriting the file took a couple of hours or more, Parker says.

SCIRun eliminates a lot of this drudgery. Parker redesigned the software so that he could simply use a computer mouse to drag and drop the electrode to its new location. Then SCIRun rebuilds only those parts of the mesh that changed—in this case, the heart. "In other places, like the lungs, the mesh doesn't change, so we do not need to recreate it," Parker says. The fact that SCIRun rebuilds only the portions that it has to saves a lot of recalculation, shortening the time it takes to tweak the simulation and see the result.

Saving time and reducing effort goes to the heart of computational steering. SCIRun allows data from an unfolding simulation to be displayed in various ways before the simulation is actually finished. By monitoring a simulation and intervening early when things aren't going right, researchers can reach their goals faster. In the heart and torso model, for example, the heart surface is color coded to represent the current's flow between the two electrodes. If, part way through a simulation, it becomes clear that the heart muscle isn't receiving enough current, the program can be paused and then restarted with the electrodes in a new location.

Top-down visualization of cerebral arteries and a brain aneurysm. Using a volume-rendering technique that allows them to view a three-dimensional dataset and isolate the interesting parts, researchers were able to make the aneurysm—the peanut-shaped object on the right side—highly visible. A series of such images helped neurosurgeons at the University of Utah Medical Center plan surgical strategies.

Out of the gate

SCIRun has been deployed to a handful of researchers around the world who are now testdriving a beta version. For example, Irina Gorodnitsky, a cognitive scientist at Alliance partner University of California, San Diego, is using SCIRun to develop a way to trace back to its source abnormal electrical activity in the brain that causes epileptic seizures—all based on electrical recordings, or EEGs, on the scalp. Gorodnitsky's success could allow surgeons to minimize the amount of tissue they must remove to end seizures.

When brain cells fire, they produce an electric field that projects outward through the skull. In her model Gorodnitsky uses that electric field to generate synthetic EEG signals. A mathematical algorithm then backtracks from scalp to source, calculating where the source must be located to generate the EEG pattern. SCIRun simplifies this process.

An epileptic seizure in the brain. This visualization shows the electrical current densities throughout the head and brain at a given instant. Red indicates areas of high electrical current while blue indicates regions of significantly less electrical current.

Geometry and electrical current flow in a human chest. This model was created to run a large-scale defribrillation simulation in SCIRun. Designed with a patient's MRI data, it shows segments of the body surface, heart, and lungs. The colored loops represent the flow of electrical current through the chest for a given instant, as computed from voltages recorded from the surface of the heart during open-chest surgery.

"I can use the graphical interface to place the sources inside the head at locations that make physiological sense," Gorodnitsky says. "Without the ability to visualize the head volume, it is really hard to position the sources blindly. We can also visualize the locations estimated by the algorithms [and compare them to] the actual locations of the synthetic sources and see how close they are."

Johnson is also gearing up to collaborate with neuroscientists at the Surgical Planning Laboratory at Brigham and Women's Hospital in Boston, a center of research on the uses of computer modeling and visualization in medicine. SCIRun could be used as a preoperative simulator for determining the safest way to excise a tumor. In addition, SCIRun could provide navigational information during the operation—say, by rendering the tumor as a solid mass suspended within a transparent view of the head and brain surface.

What's next for SCIRun? Johnson and other members of the Utah lab have founded a startup company, Visual Influence, to shepherd SCIRun into general use in science. But SCIRun's expansion outside Utah doesn't stop there.

The Alliance is supporting the group's efforts to integrate the system into the technology Grid being prototyped by the Alliance and its sister program, the National Partnership for Advanced Computational Infrastructure. While researchers run SCIRun's graphical control panel on their home machines, the background computation will tap into computing horsepower at the various sites on the Grid. If it all works as Johnson plans, SCIRun will finally put computational scientists where they belong—in the driver's seat of their own simulations.

Research on SCIRun is funded by the University of Utah Center for Scientific Computing and Imaging, the National Computational Science Alliance, and additional grants from the National Science Foundation, the Department of Energy, the National Institutes of Health, and the Utah State Centers of Excellence program.

http://access.ncsa.uiuc.edu/CoverStories/SCIRun/

For more information about this research project, see the following URLs:

http://www.cs.utah.edu/sci/
http://www.cs.utah.edu/sci/scirun/
http://www.bwh.partners.org/

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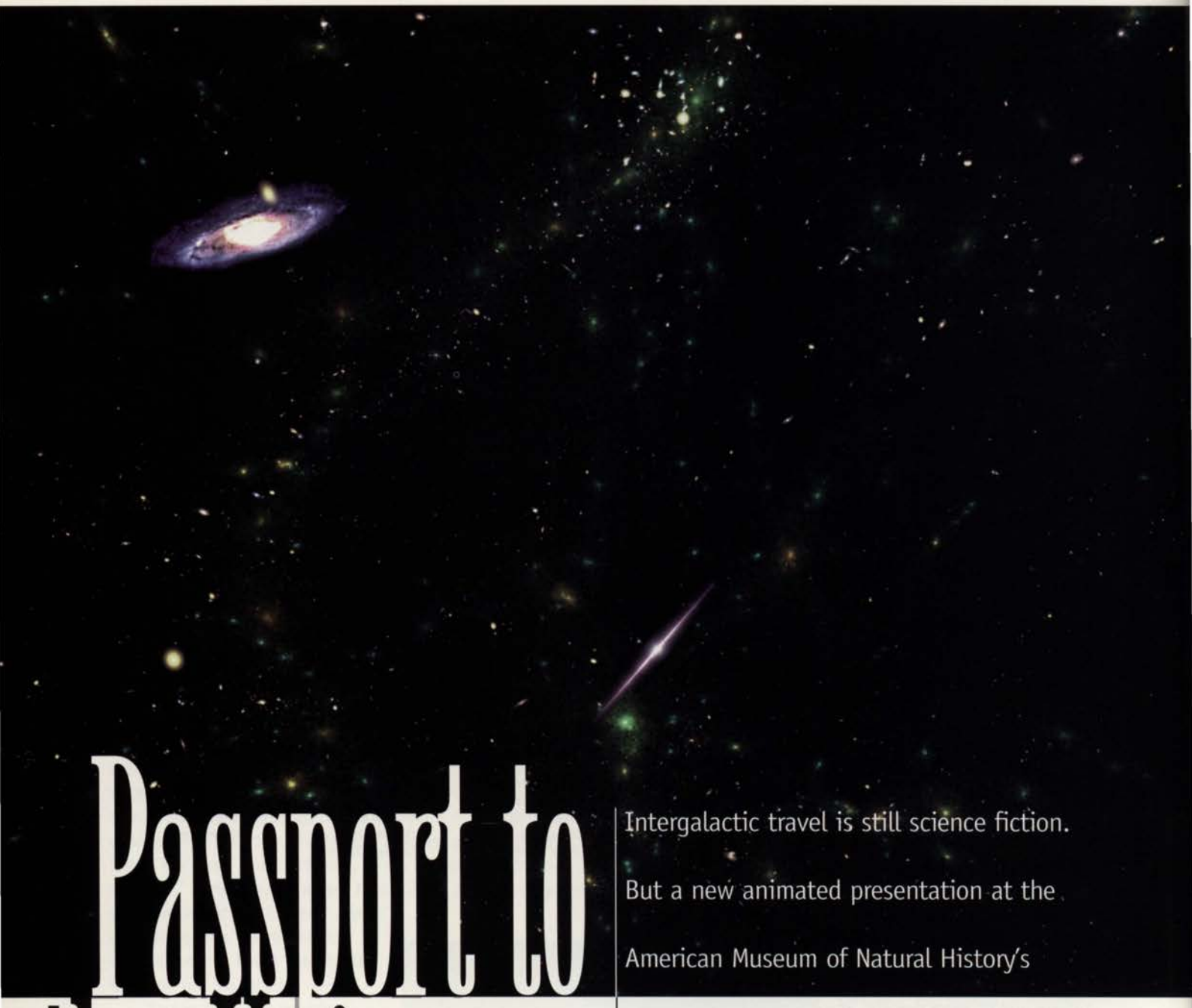


Passport to the Universe

Intergalactic travel is still science fiction. But a new animated presentation at the American Museum of Natural History's Rose Center for Earth and Space gives visitors the most accurate depiction available of what it might be like out there.

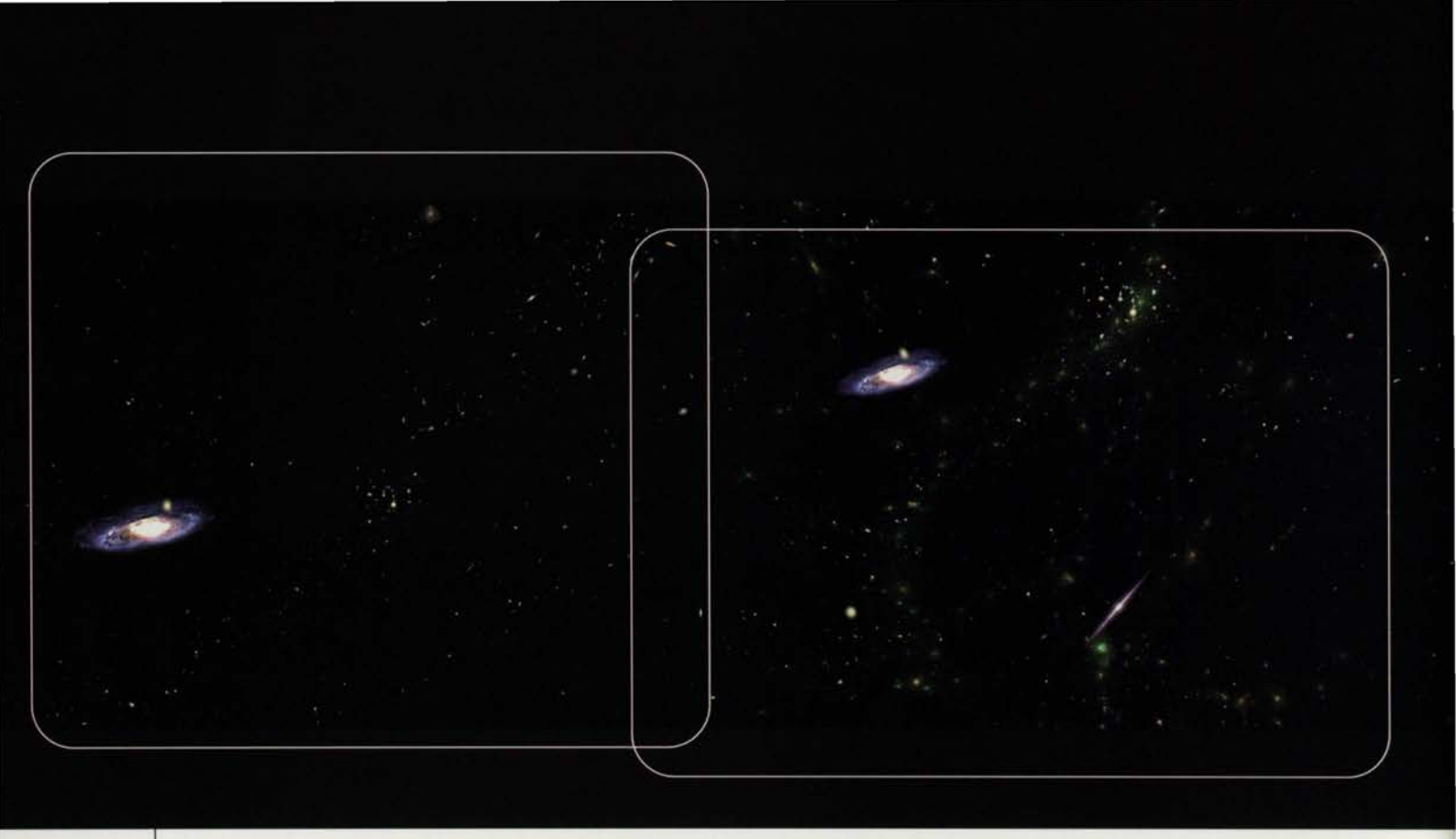
by Karen Green

When the American Museum of Natural History (AMNH) in New York opened its new Rose Center for Earth and Science in February, the Center's new Hayden Planetarium Space Theater began giving visitors an unprecedented glimpse of the wonders of the universe, thanks in part to visualizations and technologies provided by the Alliance and NCSA.

The Alliance Cosmology team, which includes AMNH, and the NCSA Virtual Director team recently helped the museum develop its first Digital Dome presentation in the unique Space Theater. The new space show, as it is called, allows audiences to fly through an astronomically accurate portion of the universe and to view simulations that show how large-scale structures, such as giant clusters of galaxies, may have formed. The digital film, called *Passport to the Universe*, is projected on the Space Theater's Digital Dome System to introduce visitors to the new and improved Hayden Planetarium. The planetarium is the centerpiece of the Frederick Phineas and Sandra Priest Rose Center for Earth and Space, a new 333,500 square-foot exhibition and research facility, which opened at AMNH on February 19.

"What we've done is use Virtual Director software to combine various datasets—both theoretical and from actual observation—to create an immersive digital display that gives people the perception they are flying through the universe, taking a tour across vast scales and seeing how our home galaxy fits into the enormous structure of the observable universe," says Donna Cox, one of the creators of Virtual Director and a professor in the UIUC School of Art and Design as well as an NCSA researcher. "This is one of the most accurate depictions of what it might be like out there—for now, it's about as close as we can get to the real thing."

Virtual Director at work. The Virtual Director software program is used to create computer aminations from simulations of scientific data. The rectangular box at center is the virtual camera. It is focused on a specific area of an astrophysics dataset. Lines connected by small squares above and to the left of the rectangle show previous camera paths through the dataset. The blue and green arrowlike lines below and to the right of the virtual camera show the current camera path. Tracked camera data—essentially a choreographed scene recorded by a user's voice and gesture—can be played back and becomes part of a digital movie made from the scientific dataset. The virtual televison in the upper right corner is used to play back the recorded data or real time tracked data.



Footage from *Passport to the Universe.* The images above show a visualization of actual astronomical objects as it transitions into a visualization of a scientific simulation. Shown in the foreground of the first image, taken from actual astronomical data, is the nearest giant galaxy to the Earth, the Andromeda galaxy. The middle images show the actual data being replaced by the simulated data. The final image shows only the simulation. The visualization of astronomical bodies is taken from a database of 35,000 galaxies and other objects in an area 700 million light years across, created by Alliance Cosmology team member Brent Tully of the University of Hawaii. The simulation into which it transitions tracks more than one billion particles as they move through a representative piece of the universe. Created by Alliance Cosmology team members Jeremiah Ostriker and Paul Bode of Princeton University, it is the largest cosmological simulation ever performed. The combined footage was created using the Alliance's Virtual Director software.

A real-time virtual universe

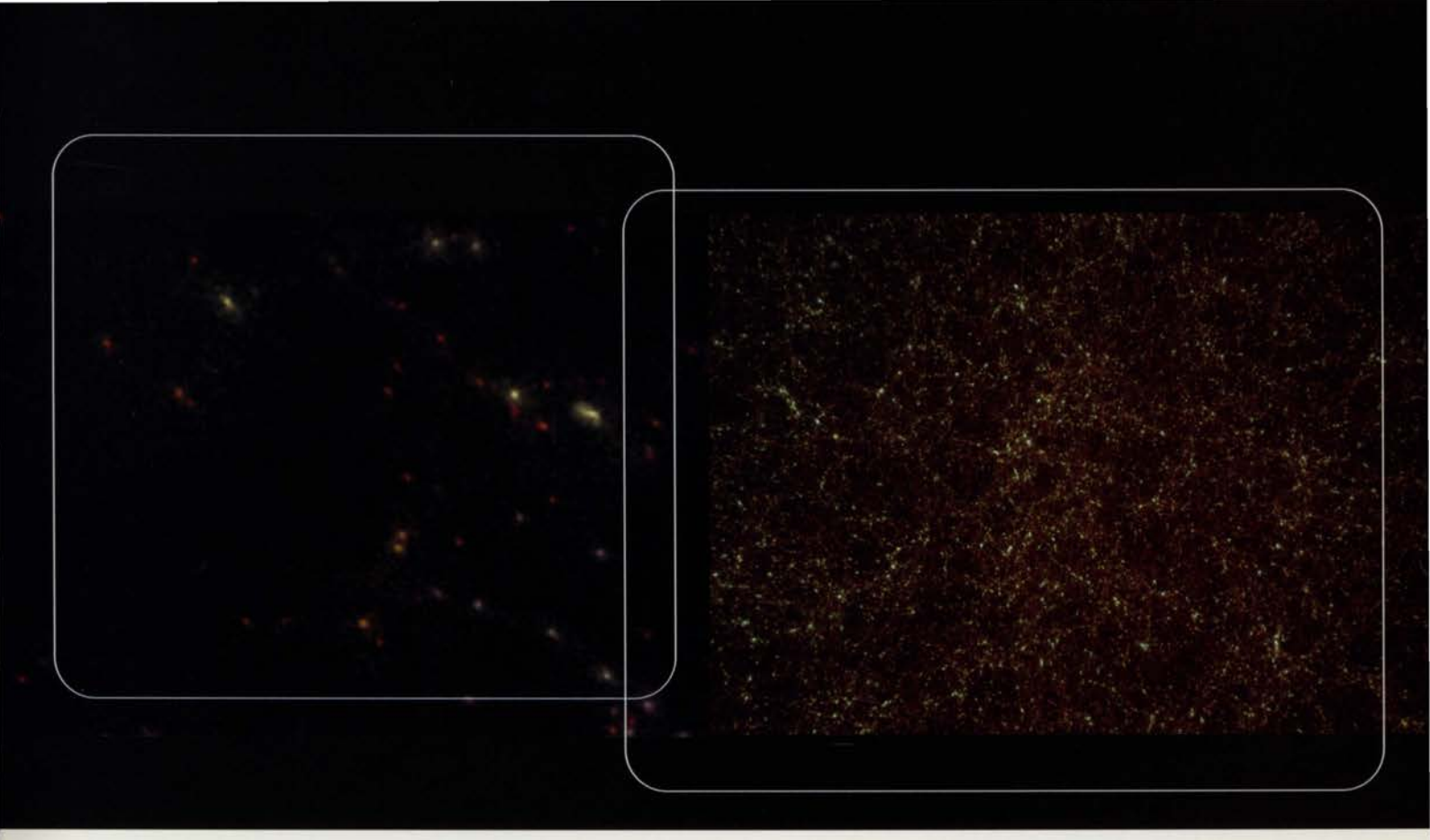
Building an astronomically accurate virtual universe requires the right tools and extensive data.

Virtual Director is a software program created by Cox, Robert Patterson of NCSA, and Marcus Thiebaux of the Electronic Visualization Laboratory at the University of Illinois at Chicago. Researchers creating visualizations from computer simulations use Virtual Director to navigate through large datasets, record and edit their movements through the data, and collaborate remotely by sharing tracker and camera data. In essence, Virtual Director lets a user navigate through a complex simulation and choreograph—or direct—with a virtual camera to create a movie.

Some of the astronomical data used to create the planetarium's new space show comes from Brent Tully, an Alliance Cosmology team member at the University of Hawaii. Tully's database of 35,000 observed galaxies represents all known galaxies within an area 700 million light years across centered at the Earth. With Virtual Director, this database can be rendered into an animation that people can fly through.

"My data represents only 1/100,000 of the potentially observable universe, but beyond this realm very little is known," says Tully. "Still, this relatively local region is rich in structural details."

Virtual Director was also used to choreograph and create animations of datasets by Cosmology team member Jeremiah Ostriker, of Princeton University, and his postdoctoral researcher, Paul Bode. Ostriker's and Bode's computer simulations track more than 1 billion particles as they move under the influence of gravity in a representative piece of the universe. Cox, Patterson, and Stuart Levy, the Virtual Director software developer at NCSA, developed innovative techniques for visualizing and integrating these datasets.



"It is enormously exciting to use the NCSA supercomputers to do something which is scientifically at the forefront, and at the same time be able to present it to the public in such a visually stunning fashion," says Ostriker, whose simulations are by far the most accurate large scale N-body simulations yet made and required more than a week to create on NCSA's 256-processor SGI Origin2000 array.

In total, the NCSA team used more than 53,000 images at a resolution of 1280 x 1024 pixels to render about four minutes of visualizations from the data provided by Tully, Ostriker, and Bode. Each full dome image consists of seven 1280 x 1024 images that have been edge blended to create a single seamless representation.

High-impact outreach

The full Digital Dome space show is a 17-minute grand opening program that combines Tully's database of the actual distribution of galaxies, Ostriker's theoretical simulations of large scale structures, visualizations from the planetarium's own Digital Galaxy database of the Milky Way, NASA data, and data from the European Space Agency's Hipparcos database. The Digital Galaxy, NASA, and Hipparcos data were rendered by a team at AMNH. The Digital Dome System uses an SGI Onyx2 InfiniteReality2 system and Trimension's display and integration technology to bring audiences the animated astronomical imagery. Final rendering of the images was done using Pixar's Renderman and StarRenderer.

"At the Rose Center for Earth and Space the goal of our premier space show is to take audienced from the earth to the edges of the observable universe, flying through real astrophysical data," says James S. Sweitzer, director of special projects for the planetarium. "NCSA and its Virtual Director team have been indispensible as our 'pilots' through the farther reaches of intergalatic space. We simply couldn't have produced this groundbreaking program without them."

The project is a high-impact way for one of the Alliance's scientific teams to reach out to a large, general audience, adds Mike Norman, an NCSA researcher and Alliance Cosmology team member who consulted on the project. "Our simulations represent some major scientific work that couldn't have even been done without the Alliance commitment to capability computing [large-scale scientific computing jobs]," he says. "It's exciting to share this work with the public through the AMNH and the Hayden Planetarium. People will be able to see what's really out there in the universe and experience phenomena that we haven't actually seen but have theorized about."

This project is supported by NCSA, the Alliance, and the American Museum of Natural History.

http://access.ncsa.uiuc.edu/Headlines/00Headlines/000201.Hayden.html

For more information about this research project, see the following URLs:
http://www.amnh.org
http://virdir.ncsa.uiuc.edu/virdir/

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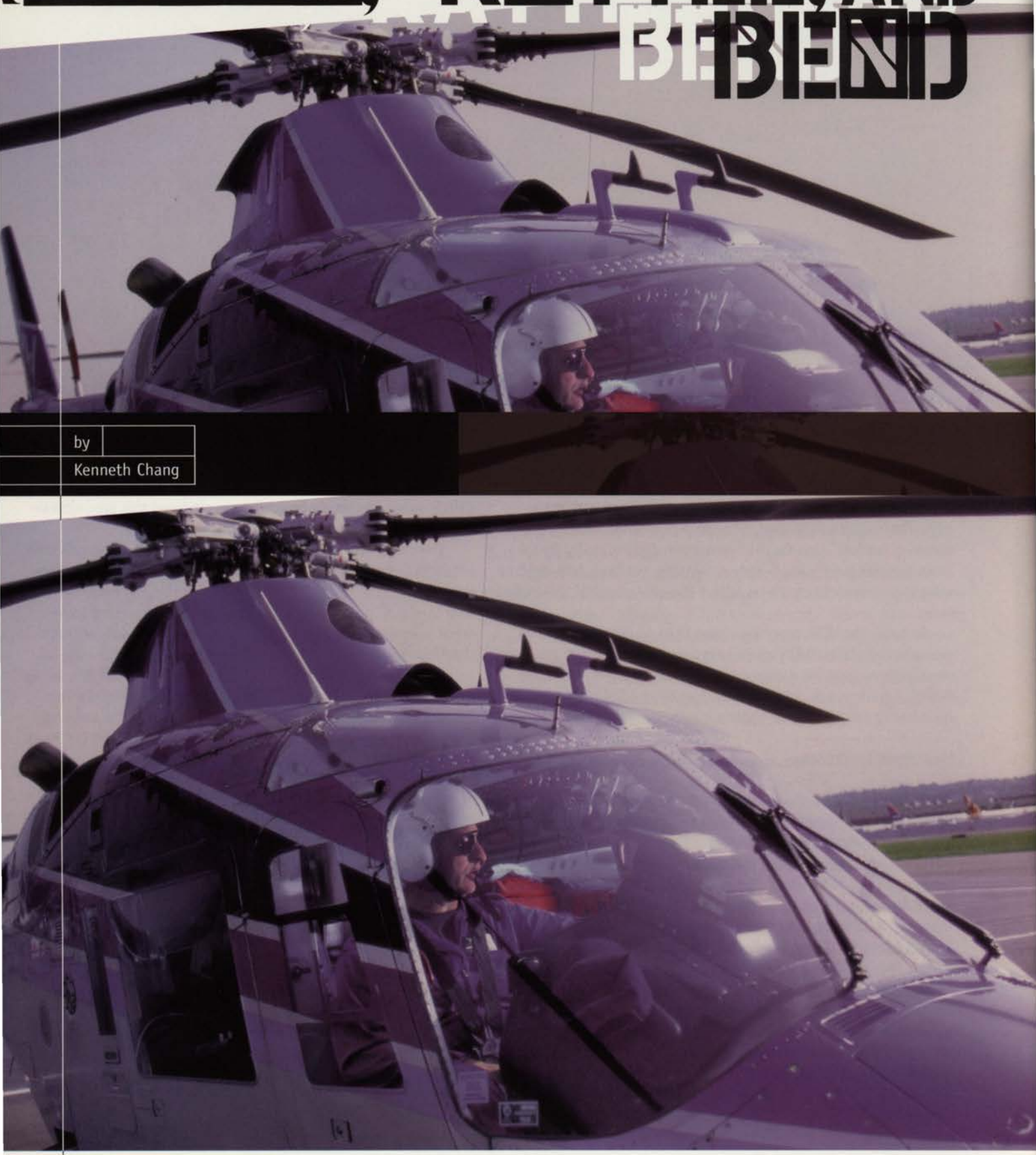
SHAKE, RATTLE, AND BEND

by
Kenneth Chang



HELICOPTERS ARE NOISY, THEY SHAKE, AND THEY ARE FICKLE IN GUSTY WINDS. BETTER COMPUTATIONAL TOOLS CAN HELP THEM FLY MORE SAFELY AND SMOOTHLY AND CARRY MORE CARGO.

Gopal Gaonkar
Florida Atlantic University

Simulating

Simulating the aerodynamics of an airplane wing, with the unpredictable whorls and eddies of turbulent air flying past, pushes the most powerful supercomputers to their limits.

Helicopter rotors present an even more difficult modeling challenge.

Wings, after all, are firmly fixed to the plane, and there are generally just two of them. Helicopter rotors, on the other hand, are essentially a bunch of wings whirling hundreds of times a minute, amplifying the vibrations, bends, and twists that occur in flight. The aerodymic interplay between the vibrating aircraft and the air around it makes for a complex mathematical tangle.

Partly because of the inherent complexities and partly because the machines didn't receive much attention until the Vietnam War, helicopters lag far behind airplanes in terms of performance and reliability. Helicopters are noisier, more difficult to fly, and give a bumpier ride than conventional aircraft.

"A helicopter is an intrinsically more complicated body compared to a plane," says Gopal Gaonkar, a mechanical engineering professor at Florida Atlantic University in Boca Raton.

Gaonkar is taking advantage of the IBM SP2 supercomputer at the Maui High Performance Computing Center, a member of the Alliance's Partnership for Advanced Computational Services, to improve the design of helicopters using Floquet analysis. The primary mathematical tool for helicopter stability investigations, Floquet analysis isn't new—it's about 125 years old. But, like other aerodynamic calculations, it takes a heap of memory and computation time, making it impractical for all but the simplest designs.

Staying trim

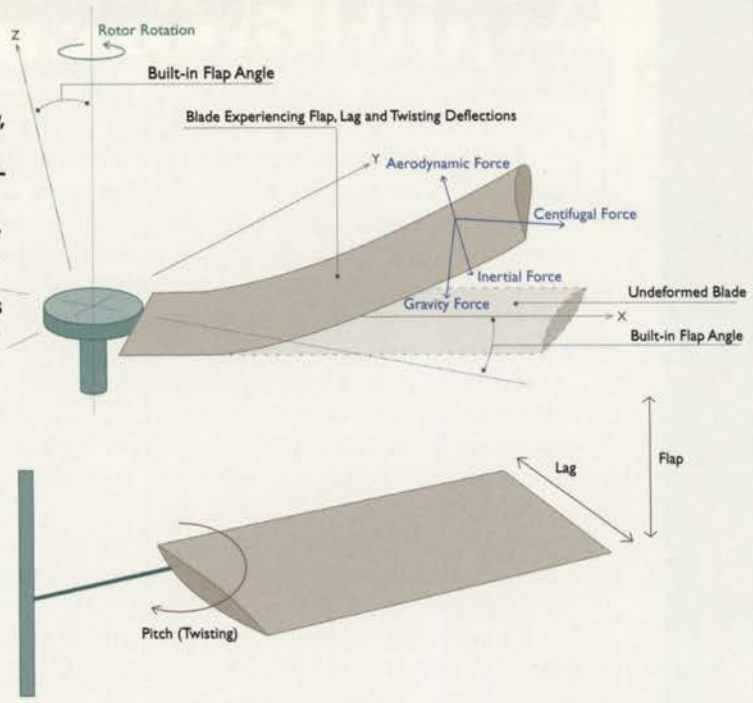
Just as your car's suspension system dampens the jolts of the road so you don't careen out of control, helicopter designers try to keep perturbations to a minimum. A pilot makes sure that the helicopter is flying steadily, or is properly "trimmed," by adjusting the rotor blades, angle of flight, and other controls. But a mistake in the design—or even factors beyond anyone's control such as a gust of wind—can disturb the aircraft's flight. The rotor blades begin to twist and bend. If left unchecked, the helicopter becomes difficult, maybe even impossible, to fly.

"If you make a small mistake in the trim analysis and the stability of the rotor design, the predicted dampening can be very off," Gaonkar says. "Then you have to come back and redo the stability analysis and put in an auxiliary damping system."

But auxiliary damping systems—which often resemble the cylinder that slows the closing of the screen door on your house—add weight to the design and cut down on the amount of payload that the helicopter can carry.

A better solution is to design rotors that are less susceptible to the instabilities in the first place. Today much rotor design still relies on small-scale models and trial-and-error. Shifting Floquet analysis to supercomputers and networked clusters of workstations, however, makes possible models and simulations that were once prohibitively complex.

Analyzing helicopter trim and stability



Forces such as gravity, inertia, centrifugal force, and aerodynamics cause stresses, known as deflections, on helicopter blades. In helicopter trim and stability analyses using Floquet theory, the blade and its deflections are represented in a three-dimensional coordinate system.

Shaving computations from the blade

Gaonkar and his collaborators have accelerated Floquet analysis in two ways. First, the researchers simply took advantage of the nature of the blades themselves and reduced the amount of computation required.

The rotor blades of a helicopter are typically identical in design and evenly spaced—take a four-blade rotor, rotate it by 90 degrees, and it looks like what you started with. Traditional Floquet analysis requires performing the calculation over the full 360 degrees of one complete revolution of the rotor blades. The team's modified Floquet technique cuts the calculation to 360/n degrees, where n is the number of blades. This step reduces the computation for a four-blade rotor, for instance, by a factor of four.

But that's still not enough to make Floquet computationally practical.

Gaonkar's team further sped up Floquet analysis by taking advantage of parallel and distributed computing. In a typical Floquet analysis simulation, each blade of the rotor is divided into a handful of segments. For each segment, the simulation tracks a dozen or more variables including position, velocity, the lift force at that point, the change in lift, and drag forces. A serial version of Gaonkar's Floquet analysis program can realistically track fewer than 100 of these state variables. Simulating more than 200—about one-third the amount considered adequate for many models—would take weeks, says Gaonkar.

A whole new ballgame

In late 1994 Gaonkar began transforming his computer code for use on parallel computers, using Message Passing Interface (MPI) software libraries, which handle the parallel computations.

At first that took effort. "The very thinking process, the very numerical process, has to be orientated to parallel computing," he says. "It's a whole new ballgame."

Within three years, though, they'd made the shift. Now Gaonkar says that running and modifying the parallel computer code is no more difficult than running traditional serial code. Instead of just 100 state variables, the parallel versions easily handle up to 1,000.

"This is a very mathematically elegant procedure and numerically reliable," Gaonkar says. "Researchers are using it for relatively small models. What we're saying here is that you can also use it for big models."

The code can be used not only on big models but also on a big variety of platforms. Gaonkar, for example, runs the code on a cluster of 13 networked workstations at Florida Atlantic University but requires the IBM SP2 at the Maui High Performance Computing Center to run the largest and most complex models.

"We are very happy with the way distributed computing has turned out," he says. "Simply put, the treatment of large and computer-intensive problems with distributed computing is no more involved than the current treatment of much smaller problems on a workstation." And that, he says, "will definitely encourage more freedom" among helicopter designers trying new configurations and designs to find better ones.

This research is funded by the Army Research Office in Raleigh, NC.

http://access.ncsa.uiuc.edu/CoverStories/Helicopters/

For more information about this research project, see the following URLs:
http://www.mhpcc.edu
http://www.me.fau.edu/

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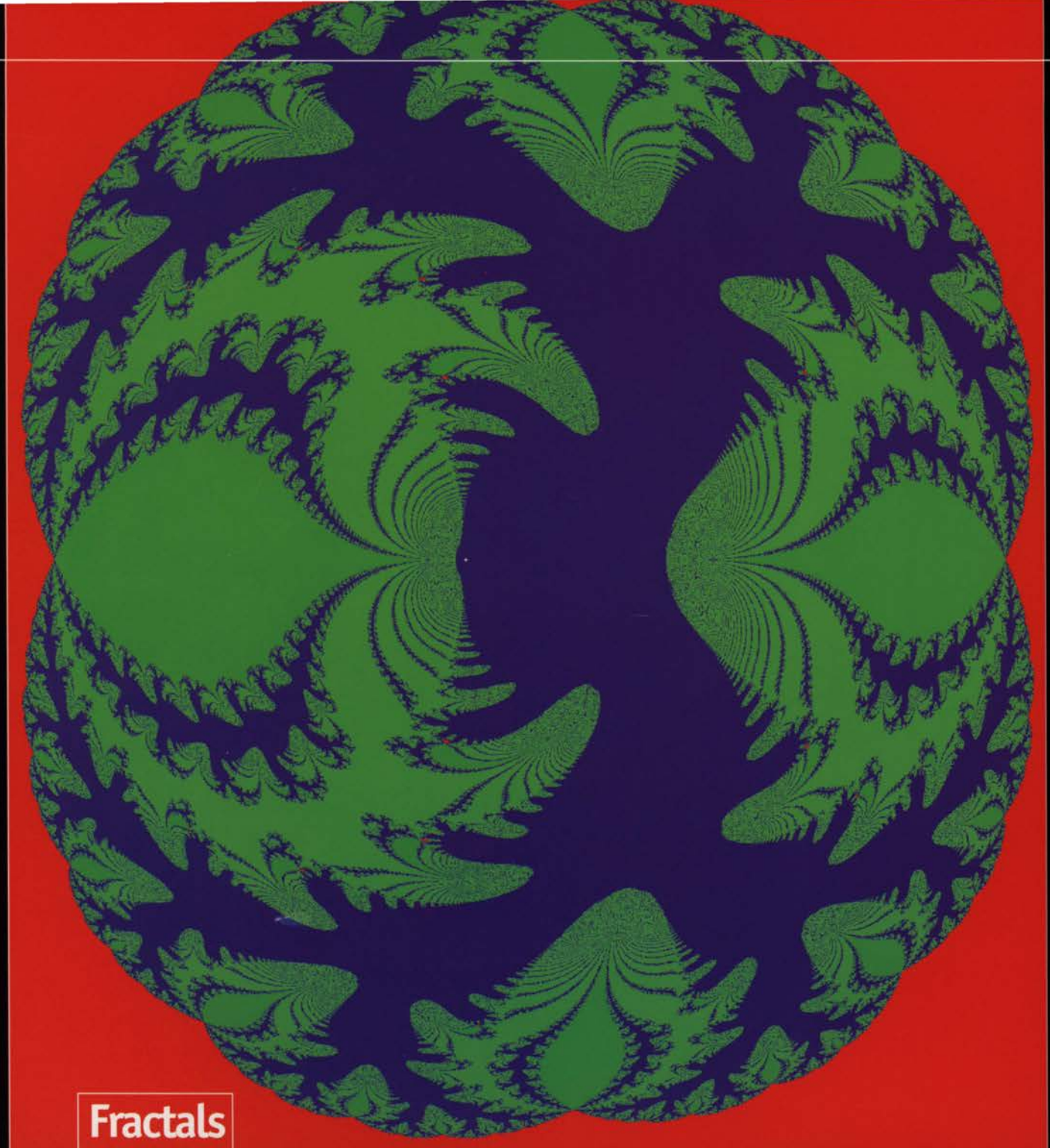

Fractals

The visualization of fractals using high-performance computing resources encourages researchers in complex dynamics—a branch of mathematics that studies the asymptotic behavior of complex analytic dynamical systems—to face new challenges.

This visualization shows the dynamics of an analytic function in the complex plane, viewed from the point at infinity in the center. The complex plane and the point at infinity can be projected to a sphere so that all points, including infinity, are then treated on an equal basis. A special projection near infinity allows researchers to bring out details without overemphasizing infinity's immediate neighborhood. The image was produced on NCSA's SGI Origin2000 supercomputer—using 64 processors and more than 40 CPU hours—by Aimo Hinkkanen, a math professor at the University of Illinois at Urbana-Champaign, Bernd Krauskopf of the University of Bristol in the United Kingdom, and Hartje Kriete of the Georg-August-Universität Göttingen in Germany.

The project particularly studies the dynamics of a certain transcendental function that can be approximated by a sequence of polynomials whose dynamical behavior converges naturally to that of the transcendental limit function. The Julia set of a polynomial of degree 1025 in such a sequence is shown in the fractal created by the boundaries of the colored regions. The approximation shows the convergence of an increasing number of attracting domains for the polynomials—the regions shown in light and dark green—to the basin of a so-called Baker domain of the limit function, where the iterates of the limit function tend to infinity. The red region beyond the outer boundary is a superattracting domain.

There are infinitely many components in the Fatou set, but only a finite number can ever been seen. The scattered red spots are tiny components of the superattracting basin, and high-performance computers are required to make them visible. More and more separate green domains merge to a single Baker domain in the limit. This convergence illustrates a fundamental difference and, at the same time, an amazing connection between the limit function and the sequence of polynomials.

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